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14. ABSTRACT We study the entanglement measured by concurrence in one-, two- and three-dimensional arrays of molecular dipoles entangled by the dipole-dipole interaction and subject to an electrostatic field. We show that the entanglement can be tuned and controlled by varying the Stark energy splitting of the $ 0\rangle$ and $ 1\rangle$ states of the molecular dipoles, the dipole-dipole coupling strength, the					
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Report Title

Final report

ABSTRACT

We study the entanglement measured by concurrence in one-, two- and three-dimensional arrays of molecular dipoles entangled by the dipole-dipole interaction and subject to an electrostatic field. We show that the entanglement can be tuned and controlled by varying the Stark energy splitting of the $|0\rangle$ and $|1\rangle$ states of the molecular dipoles, the dipole-dipole coupling strength, the temperature, and the orientation of the external electric field with respect to the array. We also developed the trace minimization algorithm for exact calculations of eigenvalues and eigenvectors of large lattices (in billions) and developed new quantum algorithms to solve complex chemistry problems such as global optimization and excited states of molecules.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

<u>Received</u>	<u>Paper</u>
08/31/2011	2.00 Mikhail Lemeshko, Mustafa Mustafa, Sabre Kais, Bretislav Friedrich. Supersymmetry identifies molecular Stark states whose eigenproperties can be obtained analytically, New Journal of Physics, (06 2011): 1. doi: 10.1088/1367-2630/13/6/063036
08/31/2011	3.00 Gehad Sadiek, Sabre Kais, Qing Xu. Dynamics of entanglement in a two-dimensional spin system, Physical Review A, (6 2011): 1. doi: 10.1103/PhysRevA.83.062312
08/31/2011	4.00 Mikhail Lemeshko, Mustafa Mustafa, Sabre Kais, Bretislav Friedrich. Supersymmetric factorization yields exact solutions to the molecular Stark-effect problem for stretched states, Physical Review A, (4 2011): 43415. doi: 10.1103/PhysRevA.83.043415
08/31/2011	5.00 Qi Wei, Sabre Kais, Bretislav Friedrich, Dudley Herschbach. Entanglement of polar molecules in pendular states, The Journal of Chemical Physics, (3 2011): 124107. doi: 10.1063/1.3567486
08/31/2011	6.00 Sabre Kais, Yong P. Chen, Qi Wei. Communications: Entanglement switch for dipole arrays, The Journal of Chemical Physics, (3 2010): 121104. doi: 10.1063/1.3366522
08/31/2011	7.00 Qing Xu, Sabre Kais, Maxim Naumov, Ahmed Sameh. Exact calculation of entanglement in a 19-site two-dimensional spin system, Physical Review A, (02 2010): 22324. doi: 10.1103/PhysRevA.81.022324
08/31/2011	8.00 Sabre Kais, Anmer Daskin. Group leaders optimization algorithm, Molecular Physics, (03 2011): 761. doi: 10.1080/00268976.2011.552444
TOTAL:	7

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

Received Paper

TOTAL:

Number of Papers published in non peer-reviewed journals:

(c) Presentations

Number of Presentations: 0.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received Paper

TOTAL:

Number of Manuscripts:

Books

Received Paper

TOTAL:

Patents Submitted

Patents Awarded

Awards

2012 Sigma Xi Research Award

2010-Present: Professor of Physics (Courtesy Appointment) Purdue
2010 Editorial Board of Papers in Physics
2008 Editorial Board of Molecular Physics
The paper "Simulated Quantum Computation of Global Minima
Jing Zhu, Zhen Huang and Sabre Kais
Molecular Physics, 107, 2015 (2009)" best paper and the cover page
of Mol. phys.

Graduate Students

<u>NAME</u>	<u>PERCENT SUPPORTED</u>	Discipline
Jing Zhu	0.50	
Sha-Hao Yeh	0.50	
Ross Hoehn	0.10	
FTE Equivalent:	1.10	
Total Number:	3	

Names of Post Doctorates

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
Qing Xu	0.10
FTE Equivalent:	0.10
Total Number:	1

Names of Faculty Supported

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Names of Under Graduate students supported

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period:	3.00
The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:.....	0.00
The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:.....	3.00
Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):.....	3.00
Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:.....	0.00
The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense	1.00
The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:	0.00

Names of Personnel receiving masters degrees

<u>NAME</u>
Total Number:

Names of personnel receiving PHDs

<u>NAME</u>
Jing Zhu
Total Number:

Names of other research staff

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Inventions (DD882)

Scientific Progress

(1) Finite-size scaling for quantum criticality using the finite-element method

Finite size scaling for the Schrodinger equation is a systematic approach to calculate the quantum critical parameters for a given Hamiltonian. This approach has been shown to give very accurate results for critical parameters by using a systematic expansion with global basis-type functions. Recently, the finite-element method was shown to be a powerful numerical method for ab initio electronic-structure calculations with a variable real-space resolution. In this work, we demonstrate how to obtain quantum critical parameters by combining the finite-element method (FEM) with finite size scaling (FSS) using different ab initio approximations and exact formulations. The critical parameters could be atomic nuclear charges, internuclear distances, electron density, disorder, lattice structure, and external fields for stability of atomic, molecular systems and quantum phase transitions of extended systems. To illustrate the effectiveness of this approach we provide detailed calculations of applying FEM to approximate solutions for the two-electron atom with varying nuclear charge; these include Hartree-Fock, local density approximation, and an "exact" formulation using FEM. We then use the FSS approach to determine its critical nuclear charge for stability; here, the size of the system is related to the number of elements used in the calculations. Results prove to be in good agreement with previous Slater-basis set calculations and demonstrate that it is possible to combine finite size scaling with the finite-element method by using ab initio calculations to obtain quantum critical parameters. The combined approach provides a promising first-principles approach to describe quantum phase transitions for materials and extended systems.

(2) Quantum algorithm and circuit design solving the

Poisson equation

The Poisson equation occurs in many areas of science and engineering.

Here we focus on its numerical solution for an equation in d dimensions. In

particular we present a quantum algorithm and a scalable quantum circuit design

which approximates the solution of the Poisson equation on a grid with error ϵ . We

assume we are given a supersposition of function evaluations of the right hand side of the Poisson equation. The algorithm produces a quantum state encoding the solution.

The number of quantum operations and the number of qubits used by the circuit is almost linear in d and $\log(1/\epsilon)$. We present quantum circuit modules together with performance guarantees which can be also used for other problems.

(3) Entanglement of polar symmetric top molecules as candidate qubits

Proposals for quantum computing using rotational states of polar molecules as qubits have previously considered only diatomic molecules. For these the Stark effect is second-order, so a sizable external electric field is required to produce the requisite dipole moments in the laboratory frame. Here we consider use of polar symmetric top molecules. These offer advantages resulting from a first-order Stark effect, which renders the effective dipole moments nearly independent of the field strength. That permits use of much lower external field strengths for addressing sites. Moreover, for a particular choice of qubits, the electric dipole interactions become isomorphous with NMR systems for which many techniques enhancing logic gate operations have been developed. Also inviting is the wider chemical scope, since many symmetric top organic molecules provide options for auxiliary storage qubits in spin and hyperfine structure or in internal rotation states

Technology Transfer